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First-principles Interatomic Potentials for Transition-Metal Aluminides

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The first-principles generalized pseudopotential theory (GPT) of transition-metal (TM) interatomic potentials[1] has been successfully extended to binary systems, including the aluminides $TM_x Al_{1-x}$. In general, the total-energy functional involves a volume term, central-force pair potentials, and angular-force many-body potentials, which are both volume and concentration dependent and include all *sp-d* and *d-d* interactions within LDA quantum mechanics. Current applications have emphasized the structural energetics of aluminum-rich 3*d* intermetallics, which appear to be well described at the pair-potential level, without angular forces. A case of special interest is the phase diagram of $Co_x Al_{1-x}$ which has recently been studied via model pair potentials[2] and *ab initio* electronic-structure calculations.[3] Preliminary GPT results reverse the incorrect prediction of a stable $Al_{12}W$ structure by the model potentials and also show good agreement with the electronic-structure results. This and other available applications will be discussed as time permits.

[1]J.A. Moriarty, Phys. Rev. B **38**, 3199 (1988).
[2]R. Phillips, et. al, Phys. Rev. B **49**, 9322 (1994).
[3]S. ögüt and K.M. Rabe, Phys. Rev. B **50**, 2075 (1994).

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